



Co-Optimization of
Fuels & Engines

Fuel-Property Impacts on Spark Ignition Efficiency, Part 1: Research Octane Number, Sensitivity, and Heat of Vaporization

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June 8, 2017



FY17 Vehicle Technologies Office Annual Merit Review

better fuels | better vehicles | sooner

Project ID: FT053

U.S. DEPARTMENT OF
ENERGY

Energy Efficiency &
Renewable Energy

VTO Management: Kevin Stork, Gurpreet Singh,
Michael Weismiller, Leo Breton

This presentation does not contain any proprietary, confidential, or otherwise restricted information.



Timeline

- Project start date: 10/1/2015
- Project end date: * 9/30/2018
- Percent complete: 56%

Budget

	FY16 Budget	FY17 Budget	FY18 Budget
VTO	\$1,610k	\$1,610k	\$1,610k

Barriers

- **Complexity:** Introduction of new fuels and vehicles involves a large number of stakeholders with competing value propositions
- **Timing:** Schedule for completing R&D and achieving market impact is extremely ambitious

Partners

Partners include 9 national laboratories, 13 universities, external advisory board, and many stakeholders and collaborators

*Start and end dates refer to three-year life cycle of DOE lab-call projects, Co-Optima is expected to extend past the end of FY18



- Internal combustion engines will continue to dominate the fleet for decades – and their efficiency can be increased significantly.
- Research into better integration of fuels and engines is critical to accelerating progress towards our economic development, energy security, and emissions goals.
- Improved understanding in several areas is critical for progress:
 - Fuel chemistry – property relationships
 - How to measure and predict fuel properties
 - The impact of fuel properties on engine performance
- This presentation is focused on LD SI combustion. MD/HD diesel, and advanced CI combustion strategies are addressed in other Co-Optima presentations.

CI: compression ignition
HD: heavy duty
LD: light duty
MD: medium duty
SI: spark ignition



- Work with researchers across Co-Optima initiative to develop organizing principals

Central Fuel Hypothesis

If we identify target values for the critical fuel properties that maximize efficiency and emissions performance for a given engine architecture, then fuels that have properties with those values (regardless of chemical composition) will provide comparable performance

Quantitative Merit Function

$$\begin{aligned} \text{Merit} = & \frac{(RON_{mix} - 91)}{1.6} - K \frac{(S_{mix} - 8)}{1.6} + \frac{0.085[ON / kJ / kg_{mix}] \cdot ((HoV_{fuel} / (AFR_{stoich} + 1)) - (415[kJ / kg_{fuel}] / (14.3[-] + 1)))}{1.6} \\ & + \frac{((HoV_{fuel} / (AFR_{stoich} + 1)) - (415[kJ / kg_{fuel}] / (14.3[-] + 1)))}{15.38} + \frac{(S_{Lmix} - 46[cm / s])}{5.4} \\ & - H(PMI - 1.6)[0.7 + 0.5(PMI - 1.4)] + 0.008^{\circ}C^{-1}(T_{c,90,conv} - T_{c,90,mix}) \end{aligned}$$

- Experimental and computation approach of the tasks in this presentation is to execute studies into whether the correct fuel properties are identified, properly weighted, and in alignment with the Central Fuel Hypothesis.



Complete constant volume ignition delay experiments and OD knock integral modeling for functional groups tested in SCE in FY16 – critical path for 18 month decision point (Zigler, Q2) **Complete.**

Complete an experimental campaign investigating autoignition propensity using the Co-Optima core fuel matrix under boosted operating conditions with and without EGR (Szybist, Q1) **Complete.**

Evaluate impact of improved air handling and higher compression ratio on operating range for Thrust I fuel blends (Edwards, Q3) **On track.**

Technical Accomplishments Outline and Budget



Title	PI	Lab	Budget
Engine Efficiency Potential of High-Octane Renewable Fuels in Multi-Cylinder Engines	Sluder	ORNL	\$550k
Multi-Cylinder Engine Simulations of ORNL Engine	Som/ Edwards	ANL/ ORNL	\$310k
SI Autoignition Behavior	Zigler	NREL	\$300k
Fuel Pressure Sensitivity and High Load EGR Dilution Effects in SI Combustion	Szybist	ORNL	\$300k
Low Speed Pre-Ignition	Splitter	ORNL	\$150k

Engine Efficiency Potential of High-Octane Renewable Fuels in Multi-Cylinder Engines



ORNL - Sluder (1/3)

Objective:

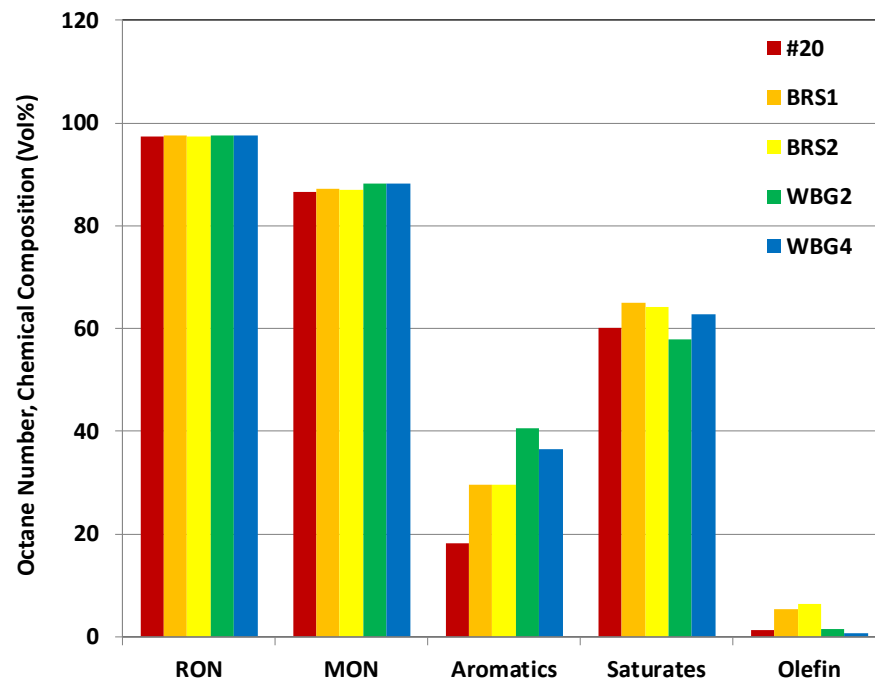
Quantify potential fuel efficiency improvements from multiple high-octane biofuel formulations while using fuels of different chemistry to test the central fuel hypothesis

Approach:

Generate performance maps with candidate fuels using a modern engine (Ford 1.6L Ecoboost) with multiple compression ratios (10:1 (stock), **12:1**, and 13:1)

Interact with Co-Optima and the Fuels Working Group (FWG) to select candidate fuels with full boiling range

Perform vehicle simulations using Autonomie to estimate vehicle energy consumption and fuel economy



Example Fuels Investigated

#20 = 20% ethanol blend

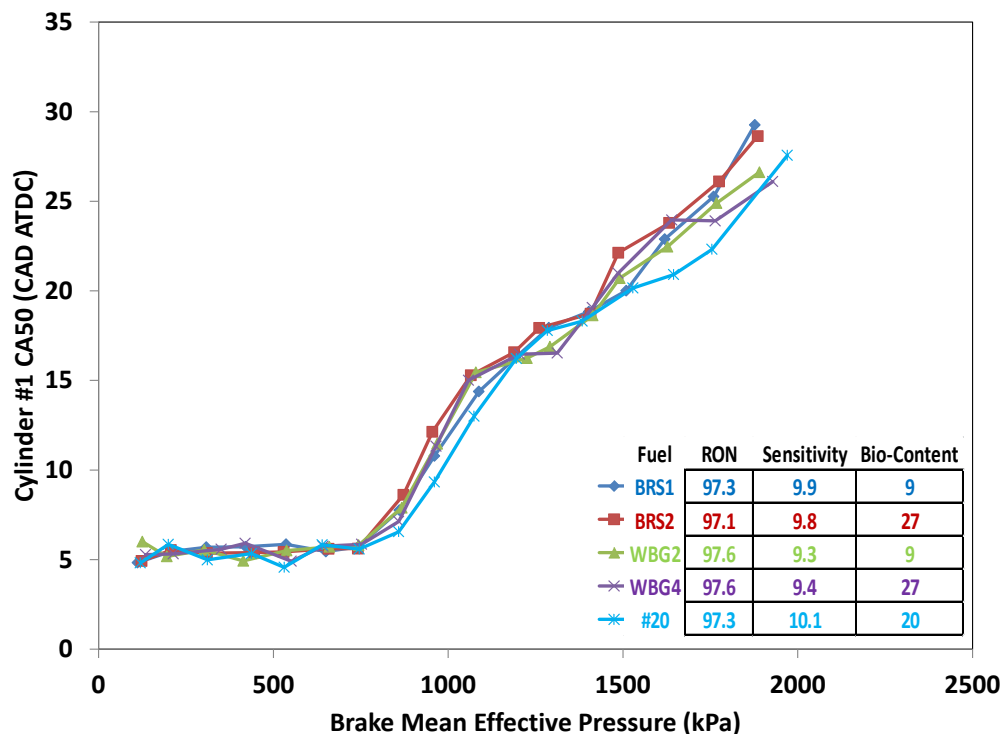
BRS = Bioreformate surrogate blend

WBG = Wood-based biogasoline blend

Matched Properties Provide Similar Performance, Aligns with Central Fuels Hypothesis



ORNL - Sluder (2/3)

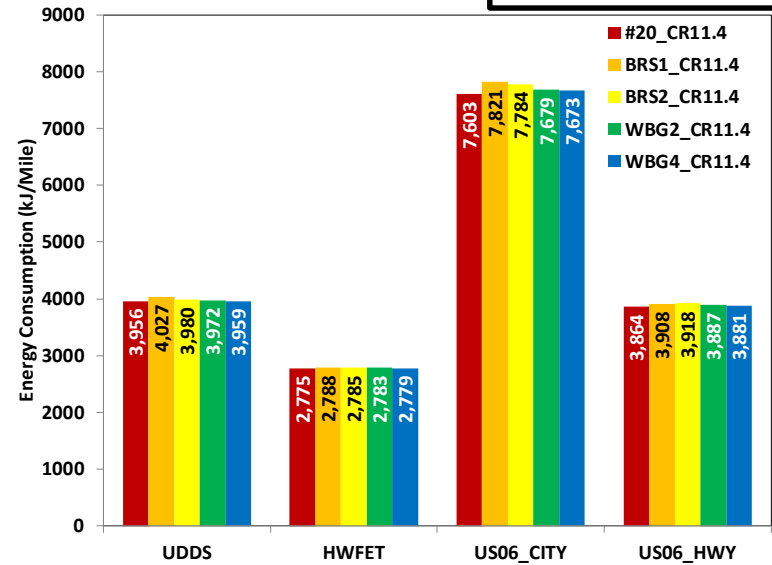
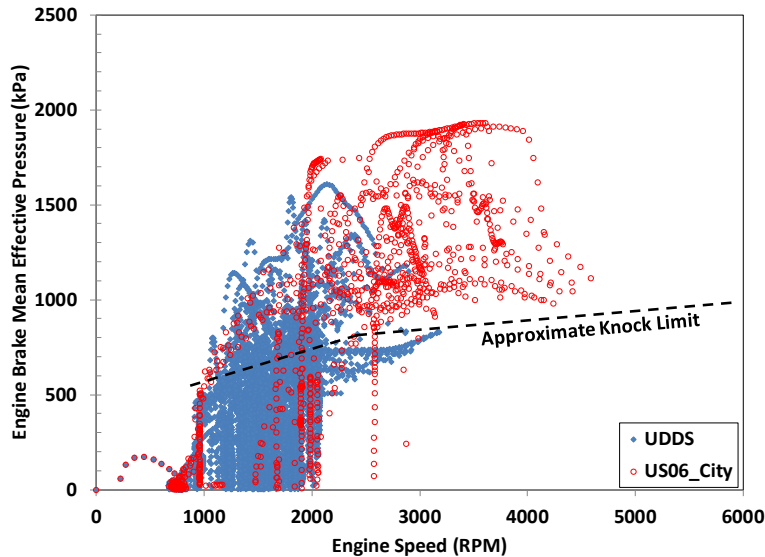


- Results affirm that under standard operating conditions, RON and sensitivity are the most important predictors of engine performance for ethanol and non-oxygenated biofuel blends
- Supports the central fuel hypothesis and provides quantification of potential benefits of multiple fuel formulations in near-term engines

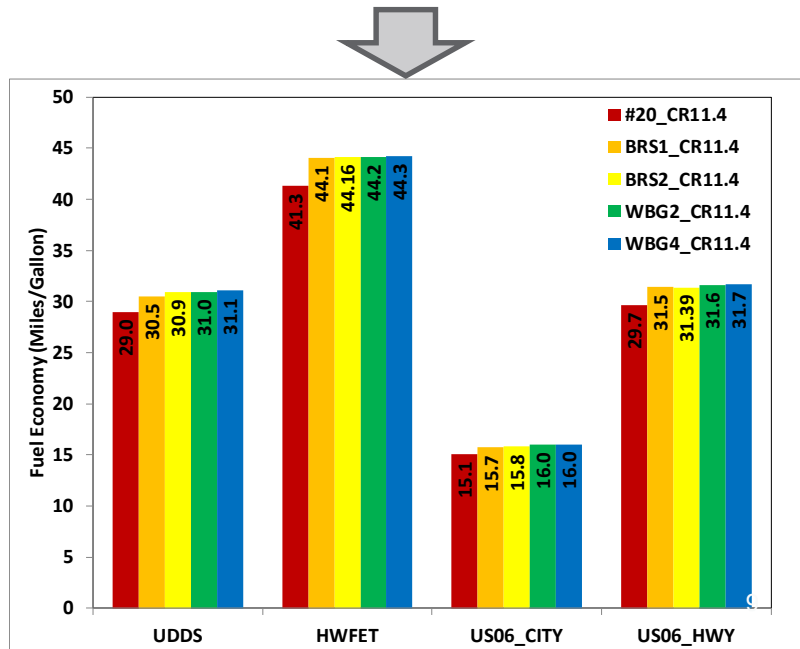
Drive Cycle is Dominant Factor in Translating Results to Modeled Fuel Economy



ORNL - Sluder (3/3)



- Drive cycle modeling with Autonomie
- US06 is more knock-limited than UDDS
- US06 consumes more energy/mile than UDDS
 - With matched fuel properties, all fuels in this fuel set consume comparable fuel energy
- As a result, modeled fuel economy is dominated by fuel energy density
 - 6% lower fuel economy for E20 blends

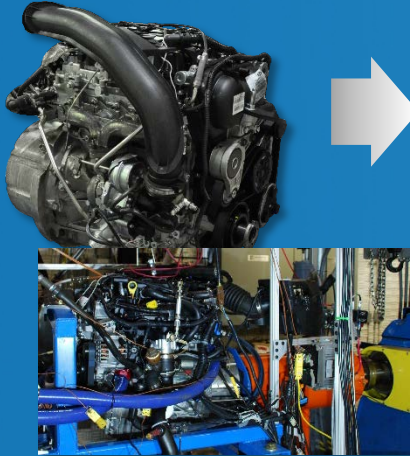


Simulation efforts expand evaluation of fuel candidates to assess potential fuel economy benefits

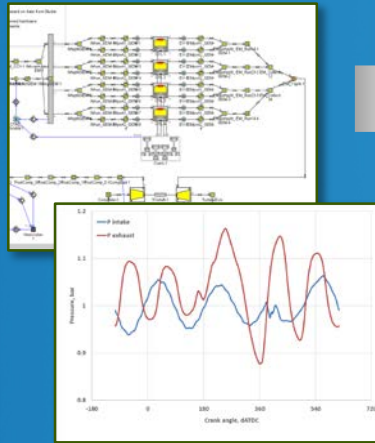


ANL/ORNL – Som/Edwards (1/2)

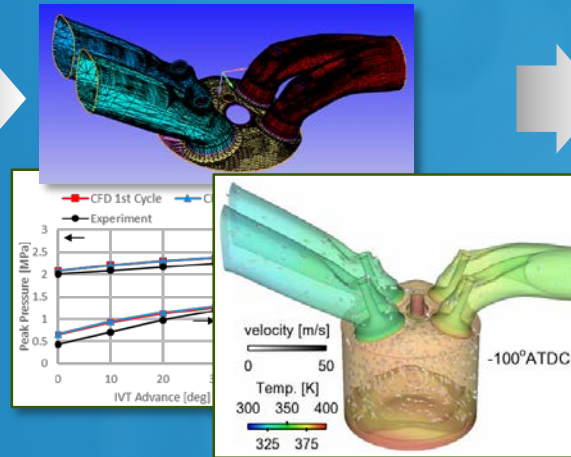
Engine experiments



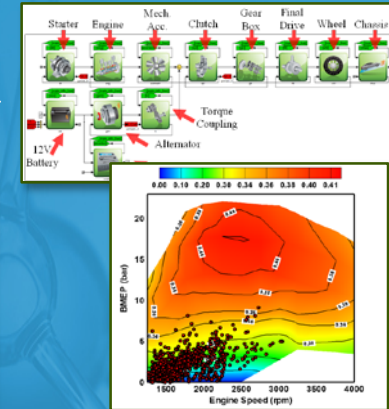
0-D simulations



CFD simulations



Vehicle-level simulations



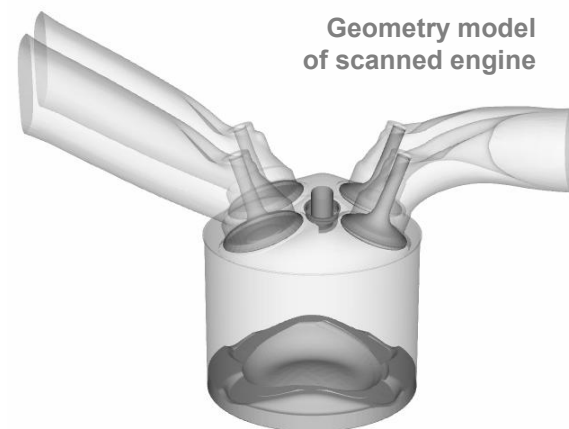
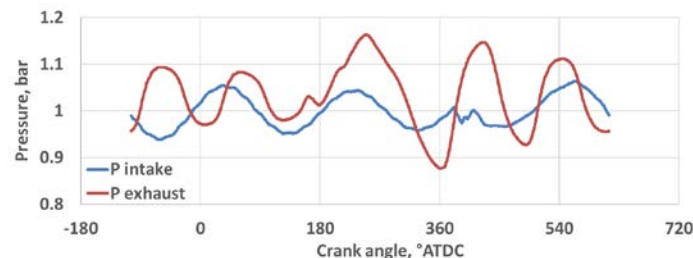
- MCE and SCE experiments at ORNL provide baseline and validation data
- Fuel property inputs and kinetic mechanisms developed by SNL and LLNL
- 0-D GT-Power simulations at ORNL...
 - Assess impact of advanced boost strategies on knock limits
 - Provide detailed BCs to CFD efforts (e.g., manifold acoustics, wall temperatures, etc.)
- CFD simulations using CONVERGE at ANL to assess and improve knock prediction
- Full fueling maps developed for candidate fuel to evaluate energy consumption and fuel economy benefits with Autonomie

Initial Model Validation Completed using SCE Motoring Data over Valve Phasing Sweep

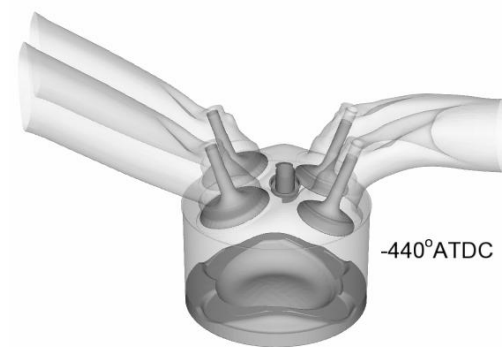
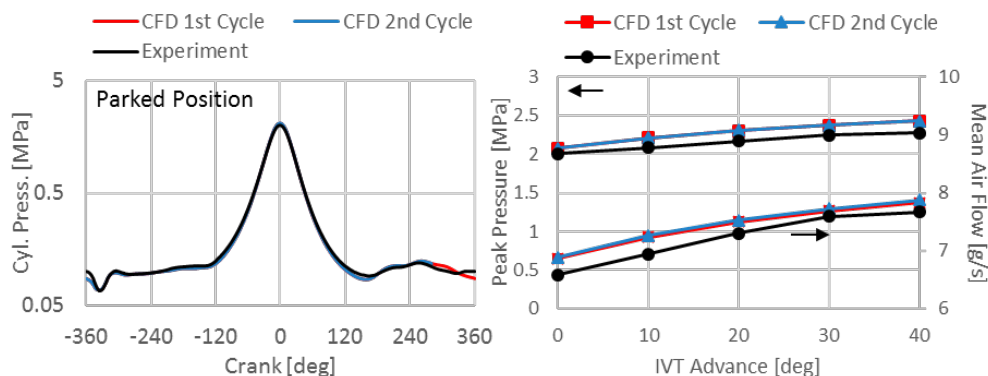


ANL/ORNL – Som/Edwards (2/2)

- Ford 1.6-L GDI geometry scanned for simulation efforts
- GT-Power simulations at ORNL provide refined BCs



- CFD simulations at ANL performed with CONVERGE
 - Re-Normalization Group (RNG) k- ϵ turbulence model, Han and Reitz wall heat transfer model
 - Minimum cell size: 0.5 mm, peak cell count: 1 million
- Predicted trends in mass air flow and peak cylinder pressure agree well with experimental observations
 - Two consecutive CFD cycles were simulated, with little variation observed
 - Errors observed over the IVT sweep within acceptable limits (<7%)



Simulation efforts of fired operation to explore onset of knock are underway

- MCE baseline validation data provided by ORNL
- Initial focus on alkylate blend with additional fuels to follow

SI Autoignition Behavior



NREL - Zigler (1/3)

Objective:

Generate high-throughput ignition delay data for candidate fuels, incorporate directly to knock integral correlations

Approach:

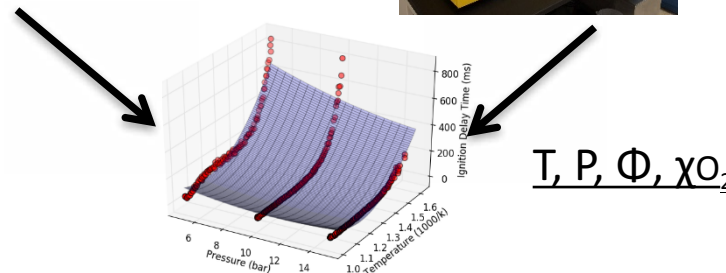
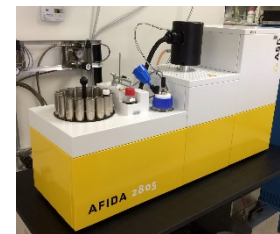
Perform temperature sweeps at several fixed pressures to provide parametric experimental ignition delay data (rather than just RON or MON), including how ignition delay increases at low temperatures in relation to increased octane sensitivity (S).

The bench-scale ignition delay data are being correlated with engine data focusing on load extension possible using spark retard with high S fuel blends.

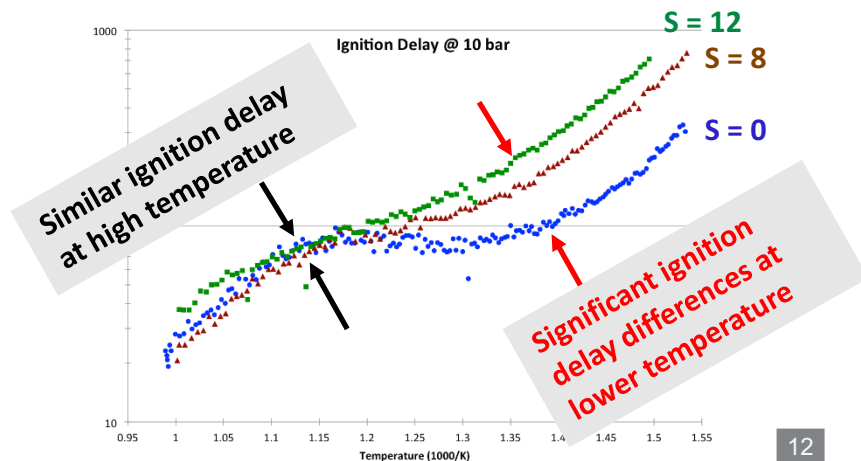
Ignition Quality Tester (IQT)



Advanced Fuel Ignition Delay Analyzer (AFIDA)



100 RON Fuels with Different S

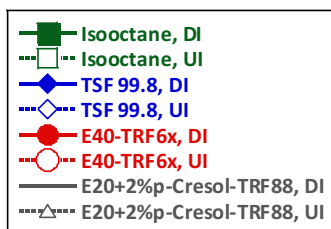
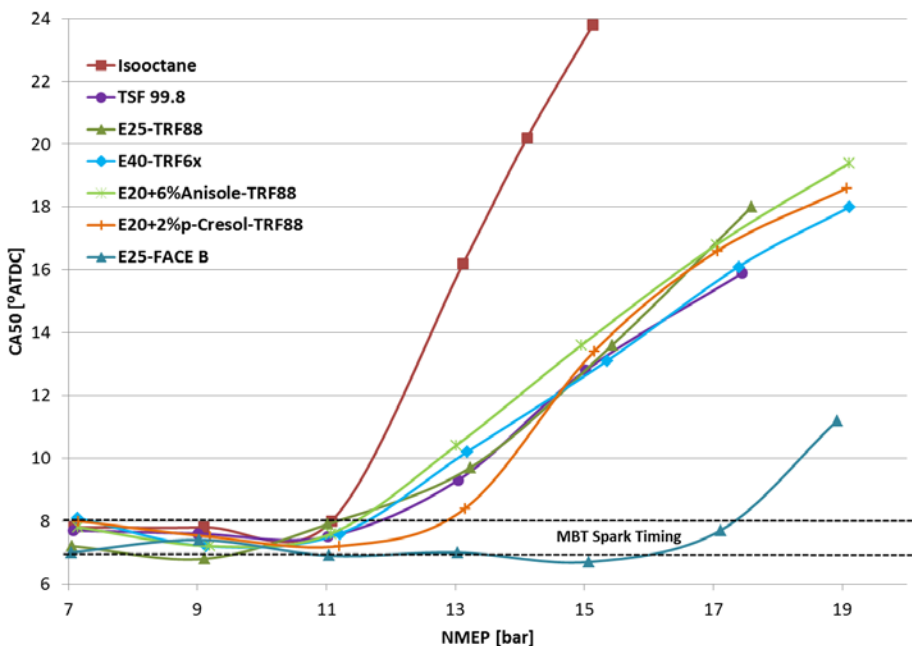


2016 AMR Results Showed Interactions Between HOV and S. Opportunity for Insight!

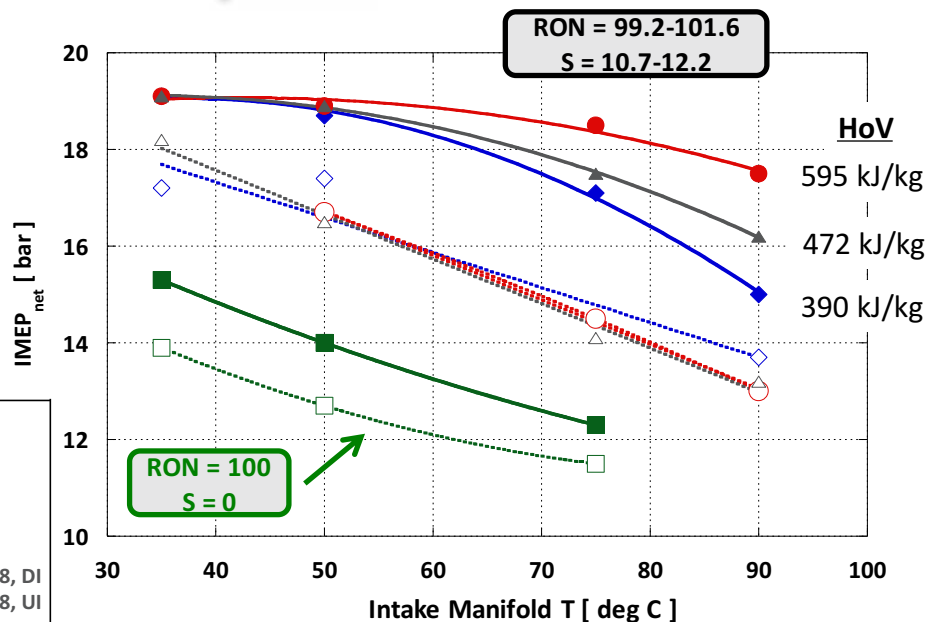


NREL - Zigler (2/3)

Single cylinder GDI engine experiments examined RON, S, and HOV effects. While HOV is captured in RON under some operating conditions, HOV can extend operating limits with elevated intake temperatures.



Knock integral modeling
in engine simulations

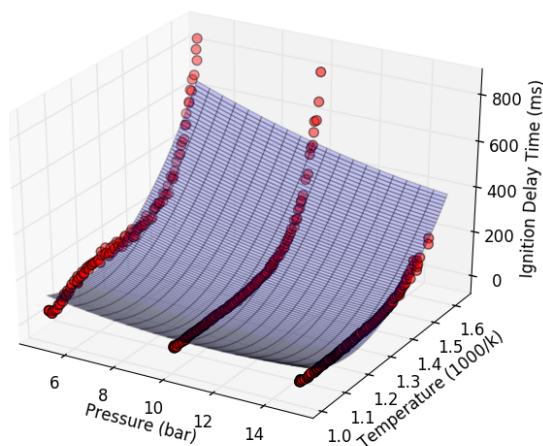


Progress: Data in Constant Volume Devices Collected, Maps Generated, Modeling In Process

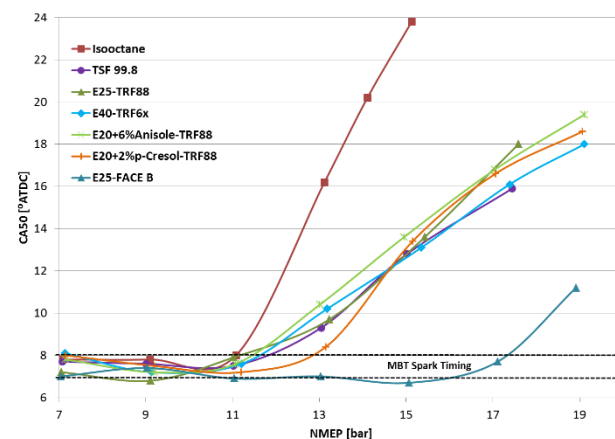


NREL - Zigler (3/3)

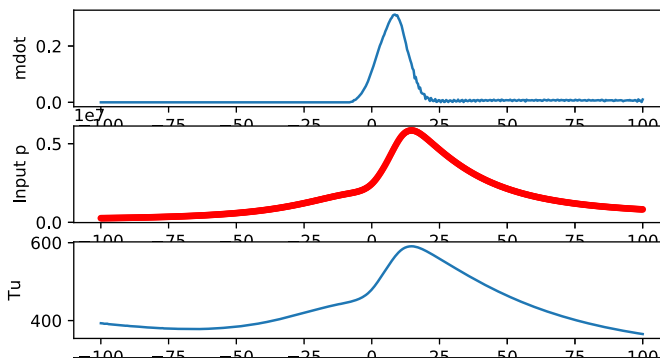
A 0D, two-zone engine simulation integrating bench-scale (IQT, AFIDA) ignition delay data in a knock integral model has been developed. This model is undergoing additional development in FY17 to use bench-scale parametric ignition delay data to predict knock in engine simulations.



Knock integral modeling
in engine simulations



GDI SCE engine data



Simulations with knock-
integral model

Bench-scale ignition delay data
for blends of Thrust I candidates

Fuel Pressure Sensitivity and High Load EGR Dilution Effects in SI Combustion



ORNL - Szybist (1/4)

Objective:

To test whether RON and MON correspond to knock-limited phasing, in adherence with the central fuel hypothesis

Approach:

Investigate knock-limited phasing under boosted conditions in a single-cylinder DI engine (GM LNF, 0.5 L displacement / cylinder)

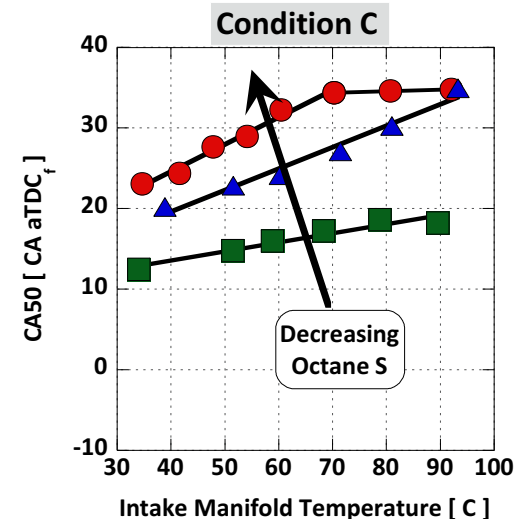
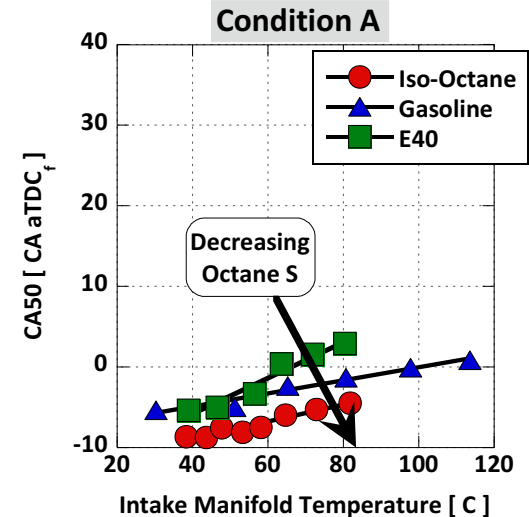
Study 1, Exploratory: 3 fuels with constant RON and varying MON, no EGR, 3 fueling rates, varying intake temperature

Study 2, Provide Data for Go/No-Go: 7 fuels (including 3 bio-blendstock candidates), 1 fueling rate, 2 intake temperatures, 3 EGR rates

At the lightest load (10 bar IMEP), lowest S provided best performance

At the lightest load (20 bar IMEP), highest S provided best performance

Study 1, Exploratory

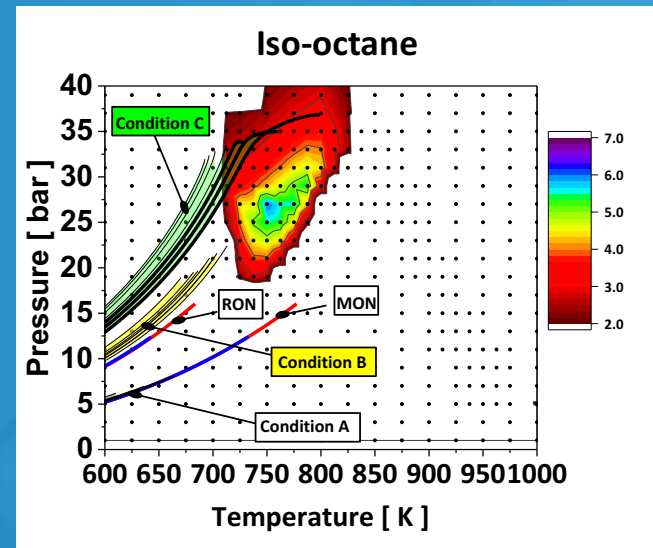
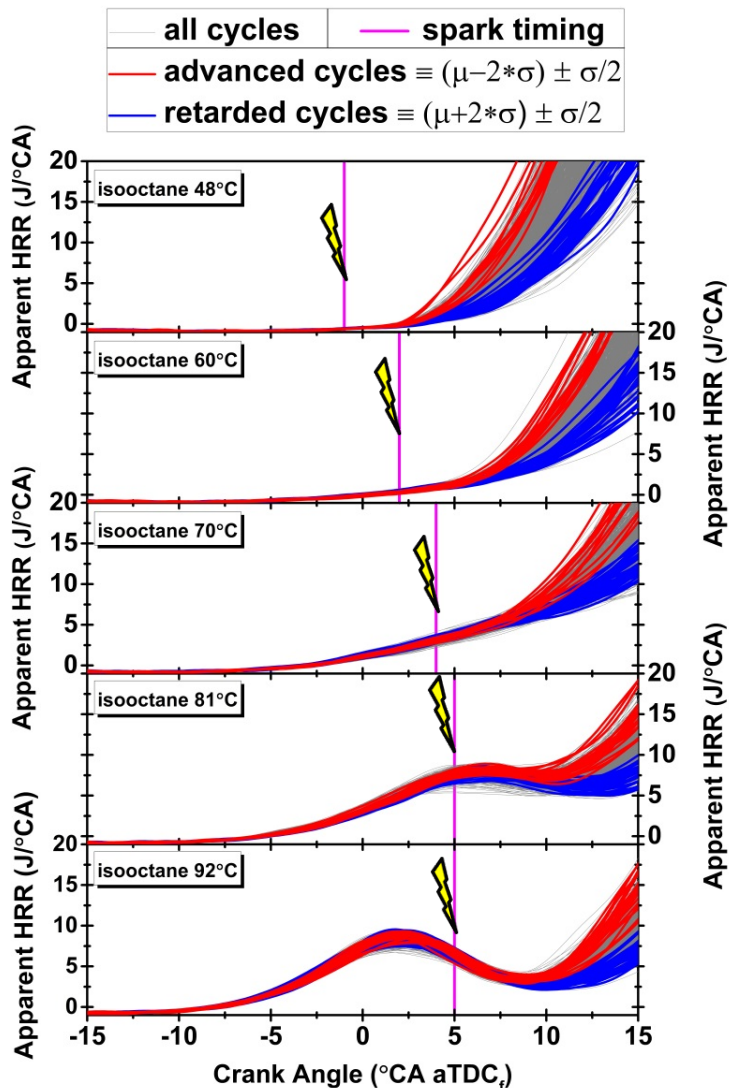


Study 1, Exploratory: Pre-Spark Heat Release Identified, Linked to Kinetics



ORNL - Szybist (2/4)

Iso-Octane



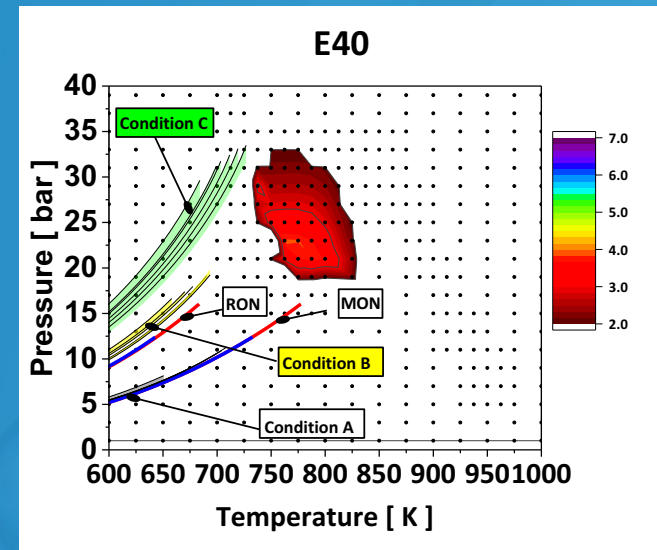
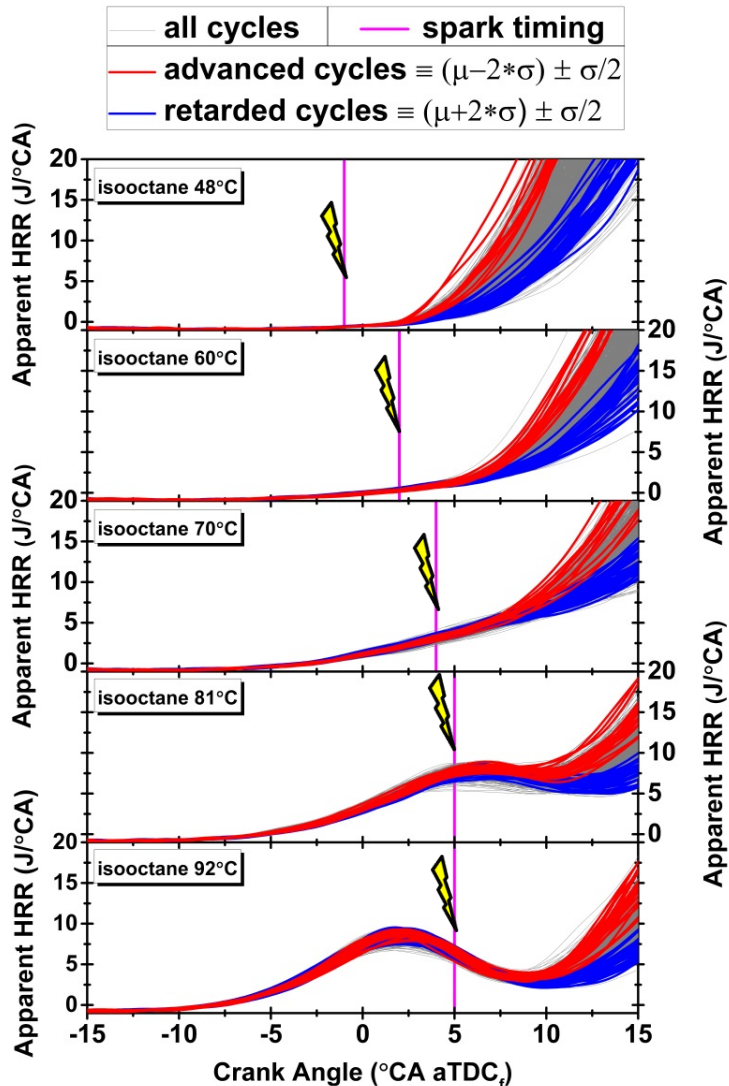
- Pre-spark heat release develops as intake temperature increases, into full LTHR with NTC behavior
- Kinetic modeling shows that under boosted “Beyond RON” conditions, these fuels enter the kinetically active island
- Full results published in *Combustion and Flame*

Study 1, Exploratory: Pre-Spark Heat Release Identified, Linked to Kinetics



ORNL - Szybist (2/4)

Iso-Octane



- Pre-spark heat release develops as intake temperature increases, into full LTHR with NTC behavior
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Study 2, Go/No-Go: Determine if Octane Index Is Predictive of Knock-Limited Phasing

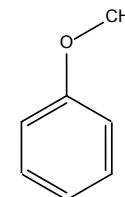


ORNL - Szybist (3/4)

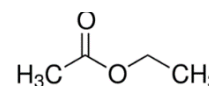
	Co-Optima "Alkylate"	Co-Optima "Aromatic"	Co-Optima "E30"	"Tier III" E10 EEE	25 mol% Methyl Butyrate Blend "MB"	25 mol% Ethyl Acetate Blend "EA"	25 mol% "Anisole" Blend
RON	97.9	98	98.3	91.8	98.1	98.5	98.8
MON	96.7	87.3	87.6	84.2	90.9	92.6	90.5
S	1.2	10.7	10.7	7.6	7.2	5.9	8.3
Aromatic	0	35.8	8.1	22.6	23 mol%	23 mol%	23 mol%
Saturates	100	65	57.1	71.2	47 mol%	47 mol%	47 mol%
Olefins	0	4.2	5	5.2	5 mol%	5 mol%	5 mol%
Ethanol	0	0	29.95	9.8	0	0	0
T10	93.1	59.4	60.7	54.6	-	-	-
T50	100.3	108.1	74.3	89.9	-	-	-
T90	105.9	157.9	155.2	157.9	-	-	-
C (wt%)	83.75	87.22	74.78	82.63	79.37	79.18	83.95
H (wt%)	15.80	13.12	13.79	13.66	12.89	12.85	12.23
O (wt%)	0	0	11.19	3.71	7.74	7.97	3.82

Fuels: Co-Optima "core" fuels, tier III cert gasoline, and 3 bio-blendstock candidates

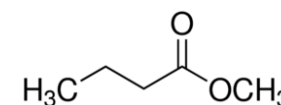
Anisole
RON = 103
S = 12



Ethyl Acetate
RON = 118
S = -2



Methyl Butyrate
RON = 107
S = 2



Operating Conditions: Constant fueling rate (14.5-19.0 bar IMEP), varying intake temperature, backpressure, and EGR

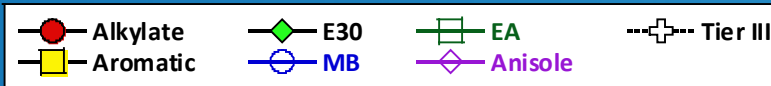
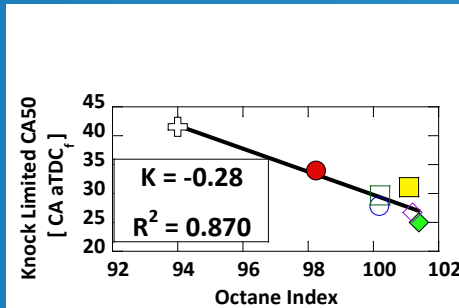
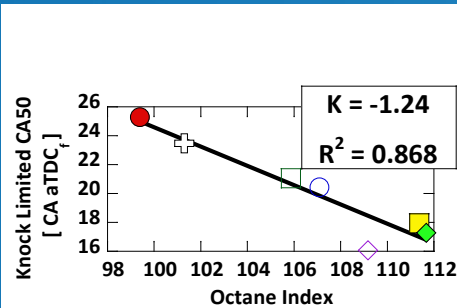
	Sweep 1	Sweep 2	Sweep 3	Sweep 4	Sweep 5	Sweep 6	Sweep 7	Sweep 8
Intake T [°C]	35	35	35	35	90	90	90	90
Manifold DP [kPa]	>20	8	8	8	>20	8	8	8
EGR [%]	0	0	10	20	0	0	10	20

Data Validates Central Fuel Hypothesis

Approach for Co-Optima Go/ No-Go



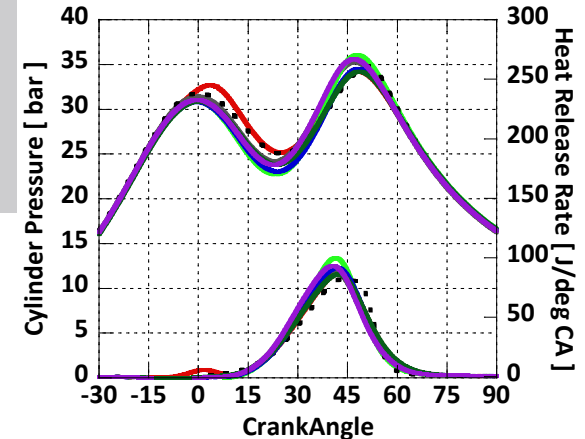
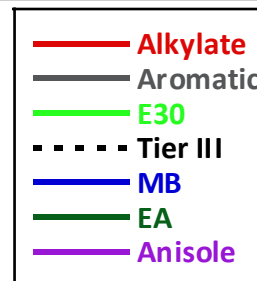
ORNL - Szybist (4/4)



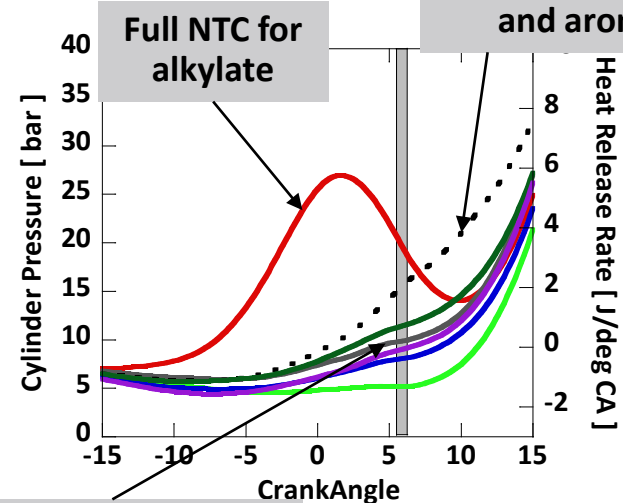
$$OI = RON - K * S$$

- Octane index includes the two most impactful terms in the merit function
- Experiments confirm that OI correlates with knock-limited phasing much better than AKI, RON, or MON
- Despite good correlation coefficients, significant outliers were observed
 - Anisole fuel blend generally out-performs OI prediction
 - Aromatic fuel blend under-performs with high intake manifold

Focusing on retarded phasing, significant differences in early combustion phases are apparent



PSHR for Tier III Fuel is between alkylate and aromatic



Low Speed Pre-Ignition



ORNL - Splitter (1/2)

Objective:

Develop a deterministic understanding of fuel composition effects on LSPI and refine merit function

Approach:

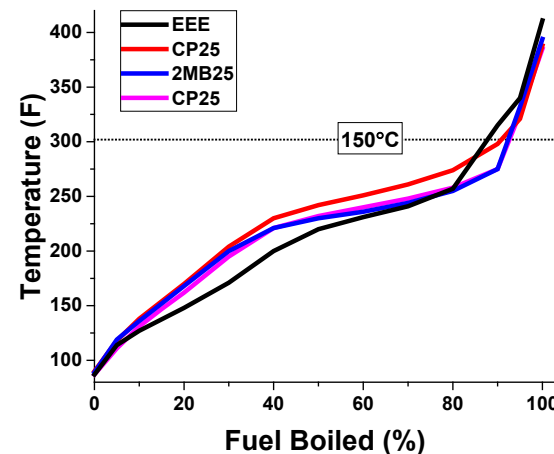
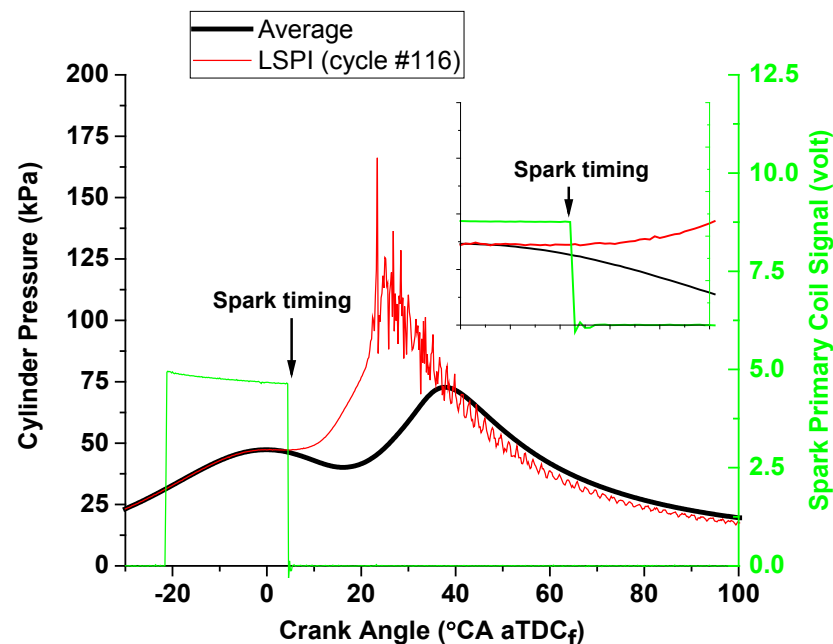
Perform LSPI experiments in single cylinder version of a modern engine with stock geometry (Ford 1.6L Ecoboost)

21 bar IMEP_g, CA50 = 36 CA aTDC_f,
9 x 20,000 cycle segments

Mix blends of 25 mass %
bio-blendstock with gasoline



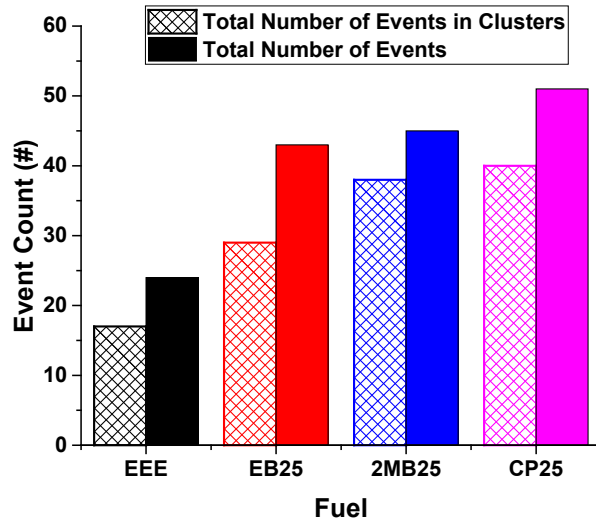
Compound	Structure	BP, °C (°F)	RON (-)	HoV (kJ/kg)
ethylbenzene		136°C (277°F)	101	394
cyclopentanone		131°C (268°F)	98	506
2-methyl-1-butanol		127.5°C (261.5°F)	101	611



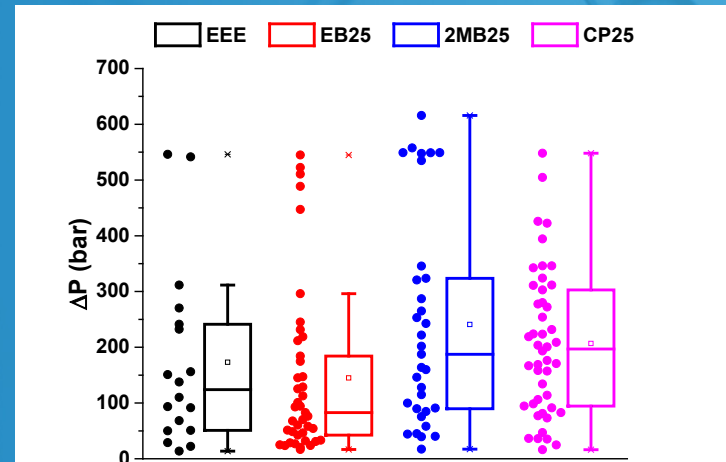
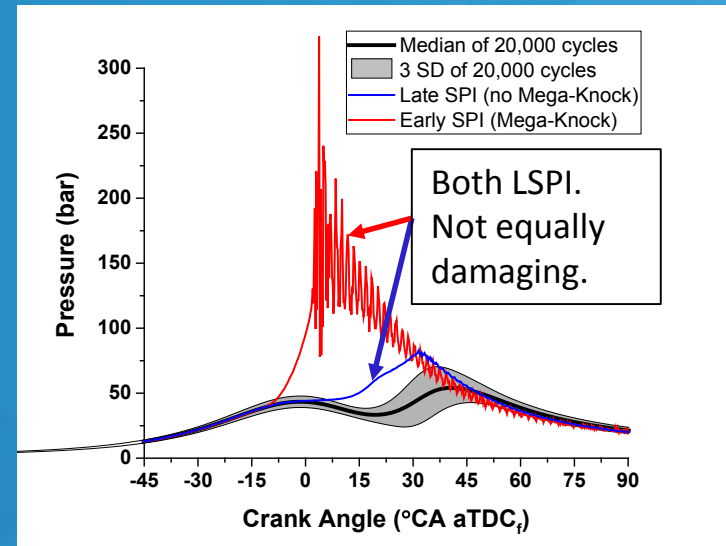
Experimental Findings Inconsistent with Literature for HC Fuels, Rethinking Merit Function Term



ORNL - Splitter (2/2)



Fuel effects also observed for LSPI severity



Cyclopentanone and methyl butanoate more prone to high severity events.

- LSPI event count lowest for baseline fuel (Tier II Certification Gasoline), but similar for all 3 candidate fuels
 - Despite lower LFM150
 - Trend is counter to literature and merit function expectations
- LFM150 approach does not accurately capture LSPI propensity, it has been removed from the merit function

Responses to Previous Year Reviewers' Comments



Note: *In 2016, 4 reviewers provided a total of 6 pages of comments to FT038, which is more than can be addressed here. Many of these comment were programmatic in nature, or specific to other areas of Co-Optima. The selected responses below were chosen on the basis of technical relevance to the projects in this presentation.*

SI engine geometry at SNL is not a good representation of Thrust I engines.

After receiving this input at the 2016 AMR, changes were made. A modeling effort presented in this presentation was undertaken to model the 1.6 L Ecoboost engine at ORNL.

Co-Optima should verify that high RON and high S fuels can result in a substantial increase in efficiency

This is part of the Co-Optima initiative. Quantifying these gains, both on an engine BTE basis and on drive cycle simulations, is the purpose of the working being led by Scott Sluder at ORNL. In addition, verifying that each fuel property with regards to the ability to increase efficiency is also part of what we're doing, and to understand the limits of if and where each fuel property breaks down.

Multiple reviewers noted that while a high level of collaboration is good, there are also concerns about the time spent on coordination.

While we acknowledge that this is an ongoing challenge, it is one that we are cognizant of. As such, continuous cost/benefit analysis of conference calls and face-to-face meetings is being conducted. There is a time penalty associated with the collaboration, but there are also many success stories within Co-Optima.

Several reviewers commented that Thrust I fuels need to be the same as the Thrust II fuels

The tasks reviewed in this presentation deal only with the spark ignition fuel needs. While Co-Optima is not restricted to a common fuel, several tasks presented during the ACI portion of Co-Optima do address this possibility.



- **Co-Optimization of Fuels and Engines** brings together expertise from across the National Laboratory system, working toward a common purpose. This effort has stakeholder engagement at a high level to ensure relevance.
 - 9 laboratories, engines, fuels, kinetics, simulation, biofuel development, LCA& TEA, market transformation
 - Monthly stakeholder engagement phone calls, industry listening days, external advisory board
- Projects presented at the semi-annual AEC program review meetings, discussed with industry and academia
- Engagement with ACEC Tech Team activities

Additional project-level collaborations with industry and academia

Sluder

Ford – Hardware and technical guidance
USDRIVE Fuels Working Group – multiple OEMs
and energy companies

Szybist

FCA

Splitter

GM
Driven Racing Oil – Custom Lubricants

Zigler

ASG Analytik – Service Gesellschaft mbH
Bosch
Ford
GM
Coordinating Research Council

Splitter

GM
Driven Racing Oils – Custom Lubricants

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Convergent Science Inc.

Remaining Barriers and Proposed Future Research for LD SI Tasks



Barrier: Understanding of Fuel Properties Falls Short in Describing Behavior in Engines

- Data collected in Co-Optima has revealed that substantial outliers exist with Octane Index, the effect of HoV appears to be dependent on operating condition, and the fuel property that was previously associated with LSPI does not correlate with LSPI.
- Future work using experimental and computational tools will be done to address these knowledge gaps
 - Work with kinetics teams to develop a more complete understanding of the Octane Index
 - Elucidate the HoV findings as they relate to knock and differences in the operating space
 - Expand the LSPI knowledgebase with regards to fuels of varying chemistry

Barrier: The Extent to which One Property can Tradeoff for Another Property is Unclear

- In exercising the merit function, a fuel with modest RON but high S can yield a higher score than a fuel with higher RON and modest S
 - Research will be done to focus on the BOB formulation

Any proposed future work is subject to change based on funding level

Summary



Relevance

Thrust I engine experiments are critical to understanding the role of fuel properties on efficiency. This information is essential to knowing how to value various fuel properties within “Co-Optima.”

Approach

Perform engine experiments that test the overarching “Co-Optima” fuel property hypothesis. Provide quantitative results that will aid in refining the Thrust I merit function. Interact with other teams within “Co-Optima” for modeling support, fuel selection, and fuels critical to the overall goal of reduced GHG emissions.

Accomplishments

- Demonstrated validity of the central fuel hypothesis for knock propensity using octane index, while showing weaknesses in some fuel properties
- Elucidated the connection between PSHR and kinetics with different fuels when boosted
- Revealed that LFV150 fuel property does not correlate to LSPI frequency, additional research needed

Collaborations

- “Co-Optima” has 9 National Labs, stakeholder engagement, and external advisory board
- Projects presented at AEC semi-annual program review, engaged with ACEC TT
- Numerous other project-level collaborations

Future Work

Co-Optima has identified several areas where the fuel property approach falls short of fully describing behavior in the engine. Experimental and computation investigations will be conducted to elucidate the behavior of fuel properties as they relate to OI, HoV, and LSPI.

Any proposed future work is subject to change based on funding level